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THE COUPLED-CLUSTER APPROACH TO QUANTUM MANY-BODY PROBLEM IN A THREE-HILBERT-SPACE REINTERPRETATION

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Abstract. The quantum many-body bound-state problem in its computationally successful coupled cluster method (CCM) representation is reconsidered. In conventional practice one factorizes the ground-state wave functions $|\Psi\rangle = e^S |\Phi\rangle$ which live in the "physical" Hilbert space $\mathcal{H}^{(P)}$ using an elementary ansatz for $|\Phi\rangle$ plus a formal expansion of S in an operator basis of multi-configurational creation operators C_j^+. In our paper a reinterpretation of the method is proposed. Using parallels between the CCM and the so called quasi-Hermitian, *alias* three-Hilbert-space (THS), quantum mechanics, the CCM transition from the known microscopic Hamiltonian (denoted by usual symbol H), which is self-adjoint in $\mathcal{H}^{(P)}$, to its effective lower-case isospectral avatar $\hat{h} = e^{-S} H e^S$, is assigned a THS interpretation. In the opposite direction, a THS-prescribed, non-CCM, innovative reinstallation of Hermiticity is shown to be possible for the CCM effective Hamiltonian $\hat{h}$, which only appears manifestly non-Hermitian in its own ("friendly") Hilbert space $\mathcal{H}^{(F)}$. This goal is achieved via an *ad hoc* amendment of the inner product in $\mathcal{H}^{(F)}$, thereby yielding the third ("standard") Hilbert space $\mathcal{H}^{(S)}$. Due to the resulting exact unitary equivalence between the first and third spaces, $\mathcal{H}^{(P)} \sim \mathcal{H}^{(S)}$, the indistinguishability of predictions calculated in these alternative physical frameworks is guaranteed.

Keywords: quantum many-body problem, coupled cluster method, *ad hoc* inner product, alternative representation spaces.

1. Introduction

The coupled cluster method (CCM) of construction, say, of the ground-state energies and wave functions of general quantum many-body systems works with virtual multi-particle excitations, and the linked-cluster nature of the contributions to the resulting estimates of measurable quantities is particularly emphasized [1] – [3]. The strategy leads, in practical calculations, to the replacement of a given, known, realistic and exact microscopic input Hamiltonian (let us denote it by the dedicated symbol H) by its lower-case isospectral reparametrization

$$\hat{h} = \Omega^{-1} H \Omega \,. \tag{1}$$

An optimal similarity-mediating transformation operator Ω is then sought in an exponential, manifestly linked-cluster form $\Omega = \exp S$. The excitations themselves are usually assumed multi-configurational, multi-indexed and generated by a complete set of mutually commuting many-body creation operators $C_j^+ \equiv (C_j^-)^\dagger$ such that, conventionally, $C_0^+ \equiv I$ and $C_0^- \equiv I$ while $S = \sum_{j \neq 0} \mathcal{S}_j C_j^+$.

Naturally, the quality of the variationally determined CCM coefficients $\mathcal{S}_j$ translates into the quality of the predicted expectation values of any operator of an observable quantity. In practice, there expectedly emerges a conflict between the precision and the costs of the results. One is thus forced to find an optimal compromise between these two requirements by introducing various approximation schemes. In our present short paper we intend to describe one possible systematic approach to the abstract formulation of approximation hierarchies.

Our considerations will be inspired by the recent progress achieved in both the formal and the applied analyses of isospectral partnerships $\hat{h} \leftrightarrow H$. In particular, we shall emphasize the innovative role played by various *non-unitary* mappings Ω, say, in their alternative time-independent or time-dependent forms as described in review papers [4] and [5], respectively.

Once a decisive simplification of the Hamiltonian is achieved by a non-unitary map $\Omega : H \to \hat{h}$, we have to start working with the less usual form $\hat{h}$ of the Hamiltonian, which becomes, in general, non-Hermitian since

$$\hat{h}^\dagger = \Omega^\dagger H (\Omega^{-1})^\dagger = \Omega^\dagger \Omega \hat{h} \Omega^{-1} (\Omega^{-1})^\dagger, \qquad \Omega^\dagger \Omega \equiv \Theta \neq I. \tag{2}$$

In our present paper we intend to reveal and describe a deeper relationship between the CCM and the abstract framework provided by the mathematical theory of Hamiltonians exhibiting the above property of quasi-Hermiticity [6], *alias* crypto-Hermiticity [7], with respect to the alternative Hilbert-space metric-operator $\Theta \neq I$,

$$\hat{h}^\dagger \Theta = \Theta \hat{h}. \tag{3}$$

In section 2 we shall explain the abstract formalism of three-Hilbert-space (THS) representation of quantum systems. We shall make use of the notation conventions of review paper [5], however, with the single, CCM-adapted exception of an interchange of the meaning of the lower- and upper-case symbols for the Hamiltonian. For the sake of clarity, Table 1 offers the explicit translation of the present notation conventions (as displayed in the first column) to the language of [5] (given in the second column). Subsequently, in section 3 an overall review of the key ideas of CCM constructions will be recalled, and their reinterpretation within the general THS scheme will be described. Section 4 will finally summarize our observations and proposals.

2. THS representation of a quantum system

2.1. Inspiration: Fourier transform

The most elementary one-dimensional harmonic-oscillator Hamiltonian

$$H^{(HO)} = -\frac{d^2}{dx^2} + x^2$$

may be recalled as one of the best known examples of an operator representing a typical quantum observable. It enters the ordinary differential Schrödinger equation

$$H^{(HO)}\psi_n^{(P)}(x) = E_n^{(HO)}\psi_n^{(P)}(x), \quad \psi_n^{(P)}(x) \in L^2(\mathbb{R}), \quad n = 0, 1, \ldots \quad (4)$$

for "physical" wave functions $\psi_n^{(P)}(x)$. The solution of this eigenvalue problem yields the well known discrete spectrum of bound-state energies $E_0 = 1$, $E_1 = 3$, $E_2 = 5, \ldots$, while the related wave functions belong to the most common Hilbert space of square-integrable complex functions of $x \in \mathbb{R}$. The argument x of the wave functions coincides with an admissible value of the position of the quantum particle in question. In other words, the $^{(P)}$-superscripted complex functions $\psi_n^{(P)}(x)$ may be interpreted as yielding the probability density of finding the particle at spatial point $x \in \mathbb{R}$.

The wave functions in question live in a physical Hilbert space $L^2(\mathbb{R}) \equiv \mathcal{H}^{(P)}$. Formally, these functions may be represented as Fourier transforms of elements of a, supposedly, "friendlier" Hilbert space, $\psi_n^{(P)} = \mathcal{F}\psi_n^{(F)}$, $\psi_n^{(F)} \in \mathcal{H}^{(F)}$. By construction, the latter space is also $L^2(\mathbb{R})$ but the physical meaning of the argument $p \in \mathbb{R}$ of the new wave functions $\psi_n^{(F)}(p)$ is different. At the same time, the primary observable (i.e., the energy) remains unchanged.

In practice, the harmonic oscillator appears equally well represented in *both* of the Hilbert spaces $\mathcal{H}^{(P,F)}$. Whenever one moves to a more complicated model, however, one may find that one of these spaces is preferable. In other words, a unitary-mapping-mediated transition to a potentially friendlier Hilbert space $\mathcal{H}^{(F)}$ should be employed whenever it appears to lead, say, to a simplification of the calculation of the energies or of the wave functions.

We only have to add here that the same recommendation remains valid even for mappings $\mathcal{H}^{(P)} \leftrightarrow \mathcal{H}^{(F)}$ which cease to be unitary. In this sense, our freedom of choosing between the upper- and lower-case Hamiltonians as expressed in Eq. (1) may prove important, say, as a source of acceleration of the rate of convergence of various numerical or variational calculations (see, e.g., their review in [4]).

2.2. Non-unitary mappings $\Omega = \exp S$

Our present text is basically inspired by the recent growth in popularity of quantum models in which the *ad hoc* non-unitary isospectral transformations

$$H \to \hat{h} = \Omega^{-1} H \Omega \quad (5)$$

perceivably simplify the Hamiltonian. Thus, Eq. (5) offers a path towards the feasibility of the evaluation of bound-state energies in complicated quantum systems via an Ω-mediated transition from a complicated "primary" Hilbert space $\mathcal{H}^{(P)}$ to a "friendlier" Hilbert space $\mathcal{H}^{(F)}$.

2.2.1. Crypto-Hermitian IBM method

One should distinguish between several non-equivalent applications of the above-outlined ideas. In one of the key references on the whole subject [4], the authors start from the knowledge of an overcomplicated H and from a qualified guess of a suitable simplification mapping $\Omega \neq \left(\Omega^\dagger\right)^{-1}$. For a persuasive illustration of the practical efficiency of such an approach the authors recalled the so-called interacting-boson-model (IBM) calculations of the spectra of heavy atomic nuclei. Using the Dyson-Maleev choice of the boson-fermion mappings $\Omega^{(\mathrm{Dyson})}$ this strategy was found to lead to successful and particularly computation-friendly forms of variational predictions of the measured energy levels [8].

The key condition of applicability of the latter IBM recipe may be seen in the feasibility of construction of the ultimate "effective" Hamiltonian $\hat{h}$ of Eq. (5). One arrives at a non-Hermitian operator in general, $\hat{h} \neq \hat{h}^\dagger$. It is worth adding that an exception may occur when the original self-adjoint Hamiltonian H accidentally happens to commute with the operator-product symmetry $\Pi = \Omega\,\Omega^\dagger$; notice that $\Pi \neq \Theta$ unless we restrict attention to the mere normal-operator mappings Ω such that $\Omega^\dagger\Omega = \Omega\Omega^\dagger$.

Whenever $\hat{h} \neq \hat{h}^\dagger$, the practical determination of the eigenvalues of the transformed Hamiltonian must remain easy and efficient. The reason is that in comparison with standard methods, one must replace the usual single time-independent Schrödinger equation by the following *doublet* of conjugate eigenvalue problems

$$\hat{h}|\Phi_n\rangle = E_n|\Phi_n\rangle, \quad \langle\tilde{\Phi}_m|\hat{h} = E_m\langle\tilde{\Phi}_m|, \quad n, m = 0, 1, \ldots \quad (6)$$

Concept	**CCM [3]**	**THS [5]**
(realistic, microscopic) initial Hamiltonian	(Hermitian) H	(Hermitian in $\mathcal{H}^{(P)}$) $\mathfrak{h}$
(non-unitary) transformation	(creation) $\exp S$	(general invertible map) $\Omega : \mathcal{H}^{(F)} \to \mathcal{H}^{(P)}$
(assumed simplified) transformed Hamiltonian	(non-Hermitian) $\hat{h} = e^{-S} H e^{S}$	$\left\{ \begin{array}{c} \text{non–Hermitian in } \mathcal{H}^{(F)} \\ \text{and Hermitian in } \mathcal{H}^{(S)} \end{array} \right\}$ $\mathfrak{H} = \Omega^{-1}\mathfrak{h}\Omega$

TABLE 1. Warning: opposite notation conventions.

using the respective action-to-the-right and action-to-the-left conventions.

Interested readers may consult review paper [5], in which a detailed discussion of further subtleties is given, first of all, for the far from trivial Heisenberg-representation-like cases in which the non-unitary mapping Ω is also permitted to vary with time.

2.2.2. $\mathcal{PT}$-SYMMETRIC MODELS

A reversal of the application of the simplification $H \to \hat{h}$ may be found promoted in the overall context of relativistic quantum field theory. In this entirely different domain of physics, Bender and his coauthors were the first who advocated an alternative philosophy of first choosing a sufficiently elementary non-Hermitian $\hat{h}$ and of postponing the reconstruction of the overcomplicated selfadjoint operator H, sometimes even indefinitely.

The initial move is due to Bender and Boettcher, who published, in 1998, an influential letter [9]. In this work they noticed that certain elementary non-Hermitian toy-model operators $\hat{h}$ appeared to possess real and bound-state-like spectra, which were discrete, non-degenerate and bounded from below. In 2001, their observations were rigorously proved while, a few years later, some of these results were also complemented by approximate reconstructions of the necessary metric operator(s) $\Theta = \Theta(\hat{h})$ (cf., e.g., review [10] for details).

On a model-independent level these developments finally resulted in a fully consistent innovative THS strategy in which one *starts* from a sufficiently elementary lower-case (i.e., non-Hermitian) candidate for a "realistic-model" Hamiltonian $\hat{h} \neq \hat{h}^{\dagger}$. Under a number of assumptions (cf., e.g., reviews [4, 11–13]) one is then able to *re-construct* a suitable Hilbert-space mapping $\Omega = \Omega(\hat{h})$ and, via Eq. (1), also a self-adjoint, textbook-compatible isospectral avatar $H = H^{\dagger}$ of the Hamiltonian living in $\mathcal{H}^{(P)}$. In other words, from the initial knowledge of a quantum-dynamics-determining operator $\hat{h}$ one is able to reconstruct, in principle at least, one or several tractable, textbook-compatible phenomenological quantum-mechanical and/or field-theoretical models.

Naturally, the initial choice of Hamiltonian $\hat{h} \neq \hat{h}^{\dagger}$ acting in $\mathcal{H}^{(F)}$ should guarantee that the pair of Schrödinger Eqs. (6) remains sufficiently easily solvable. This requirement is not so easily satisfied. In practice people usually accept various independent and additional simplification assumptions, therefore. Among them, a truly exceptional status belongs to the so called $\mathcal{PT}$-symmetry assumption or, more generally, to the assumption of the so called pseudo-Hermiticity property of $\hat{h}$ (interested readers should consult, e.g., review [12] for more details).

2.2.3. TOWARDS THE COMPLEX ENERGY SPECTRA.

A third and still different implementation of the non-Hermitian-observable ideas is much older than the previous two. It may be traced back to the traditional model-space projection technique of Feshbach in which one of the non-unitary mappings Ω and Ω^{-1} is chosen as a projector so that the other one cannot exist. It is well known that the resulting simplified effective Hamiltonians are restricted to a subspace while becoming energy-dependent in general. In this sense, Feshbach's effective Schrödinger Eqs. (6) are *de facto* nonlinear.

Such a case certainly lies outside the scope of our present considerations. Still, it is worth noting that there has recently emerged a number of papers in which the authors pointed out the existence of numerous links between the latter studies of resonances (i.e., of the quantum Hamiltonians possessing complex spectra) and their above-mentioned real-spectrum alternatives. Interested readers may consult, e.g., monograph [14] to see a number of newly discovered connections between the physics of Hermitian and/or non-Hermitian effective Hamiltonians and the related mathematics, which recommends, say, the use of the concepts of the Kato's exceptional points, etc.

One should also point out that even in the recent physics-based and experiment-oriented studies of the real-spectrum pseudo-Hermitian and $\mathcal{PT}$-symmetric models there has been a definite increase of interest in the interdisciplinary applications of the THS-related concepts of the spontaneous $\mathcal{PT}$-symmetry breakdown and/or explanations of the exceptional-point-related phase-transition mechanisms connected with the loss of the reality of the spectrum (cf., e.g., the recent quantum-theory-related review paper [15], or a sample

[16] of a successful transfer of these ideas even beyond the realm of quantum theory itself).

3. THS interpretation of CCM constructions

Having passed through the extensive list of motivating considerations we are now getting very close to the key purpose of our present paper. For the construction of a concrete backward mapping $\Omega = \Omega(H)$ in the CCM context we see that we might accept directly some of the THS constructive techniques. Naturally, in the CCM framework we encounter the possibility of extending its philosophy and its range beyond the ground-state constructions. For this purpose we may decide to experiment with various THS-inspired alternatives to the basic (bi-)variational CCM ansätze.

In an introductory step let us return, therefore, to the IBM-motivated version of the THS approach, in which one assumes a full knowledge of the realistic, albeit prohibitively complicated, Hamiltonian $H = H^\dagger$, defined in some microscopic physical Hilbert space $\mathcal{H}^{(P)}$. A qualified guess or construction of Ω will be then vital for the success of computations, i.e., first of all, for the success of the practically tractable construction and solution of the pair of Schrödinger Eqs. (6).

3.1. Brief introduction to CCM constructions

In the CCM context, the generic, Dyson-inspired non-unitary mapping $\Omega^{(CCM)}$ has traditionally been considered in the specific linked-cluster form of an exponential operator $\Omega^{(CCM)} = \exp S$. In the literature (cf., e.g., [17] with further references) one may find a huge number of practical applications of the CCM strategy by which the ground-state wave functions are sought in the form of products

$$|\Psi\rangle = e^S|\Phi\rangle. \tag{7}$$

The ket vector $|\Phi\rangle$ represents here a normalized state (usually called the model state or reference state), intended to be employed as a cyclic vector with respect to a complete set of mutually commuting multi-configurational creation operators $C_\jmath^+ \equiv (C_\jmath^-)^\dagger$. Our use of the special symbol $\jmath$ for the index indicates that this is a multi-index that labels the set of all many-particle configurations. In other words, states of the many-particle quantum system in question can be all written as superpositions of basis states $C_\jmath^+|\Phi\rangle$.

Variational eigenkets (7) of the many-body self-adjoint Hamiltonian $H = H^\dagger$ are conveniently written in terms of the specific CCM *operator* ansatz

$$S = \sum_{\jmath\neq 0} \mathcal{S}_\jmath C_\jmath^+. \tag{8}$$

The fundamental CCM replacement (7) of an unknown vector $|\Psi\rangle$ by an unknown operator S is very well motivated from several independent points of view. One of the motivations is inherited from Rayleigh-Schrödinger perturbation theory, in which, at a certain stage of construction, the *operator* Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ in question is replaced by its *single* bra-vector projection $\langle 0|H|\Psi\rangle = E\langle 0|\Psi\rangle$ or, more generally, by a *finite* multiplet of such projections $\langle 0_j|H|\Psi\rangle = E\langle 0_j|\Psi\rangle$.

The key advantage of such a reduction lies in the possibility of a variationally optimal choice of the bra-vectors $\langle 0_j|$. By contrast, the property of the Hermiticity of Hamiltonian H becomes, to a large degree, irrelevant. Thus, one transfers this experience to the CCM context by introducing a complementary, formally redundant concept of left-action variational eigenvector $\langle\tilde\Psi|$ of H.

The nontrivial difference between the tilded and untilded eigenvector $|\tilde\Psi\rangle$ and $|\Psi\rangle$ is motivated by the possibility of introducing an additional set $\{\tilde{\mathcal{S}}_\jmath\}$ of free parameters in the bra-vector

$$\langle\tilde\Psi| = \langle\Phi|\tilde S\mathrm{e}^{-S}; \qquad \tilde S = I + \sum_{\jmath\neq 0}\tilde{\mathcal{S}}_\jmath C_\jmath^-. \tag{9}$$

Together with the conditions of completeness of the basis

$$\sum_\jmath C_\jmath^+|\Phi\rangle\langle\Phi|C_\jmath^- = I = |\Phi\rangle\langle\Phi| + \sum_{\jmath\neq 0} C_\jmath^+|\Phi\rangle\langle\Phi|C_\jmath^-, \tag{10}$$

and together with the usual properties of the creation and annihilation operators,

$$C_\jmath^-|\Phi\rangle = 0 = \langle\Phi|C_\jmath^+; \quad \forall\jmath\neq 0 \tag{11}$$

and

$$[C_\jmath^+, C_J^+] = 0 = [C_\jmath^-, C_J^-] \tag{12}$$

we arrive at the standard version of the CCM formalism, in which one currently employs approximations which do not make use of the manifest Hermiticity of the original eigenvalue problem. Such approximations may entail keeping only a physically motivated subset of the multi-indices $\jmath$ in the otherwise exact expansions of the correlation operators S and $\tilde S$ in Eqs. (7)–(9).

As an immediate mathematical consequence, the CCM Schrödinger equation for ground state acquires the two different and mutually non-conjugate alternative forms

$$\begin{aligned} \hat h|\Phi\rangle &= E|\Phi\rangle, \\ \langle\Phi|\tilde S\,\hat h &= E\langle\Phi|\tilde S, \\ \hat h &= \mathrm{e}^{-S}H\mathrm{e}^S. \end{aligned} \tag{13}$$

Obviously, once the two sets of coefficients $\{\mathcal{S}_\jmath\}$ and $\{\tilde{\mathcal{S}}_\jmath\}$ are determined, all the ground-state properties of the many-body system in question may be considered as known.

The ground-state expectation value of any given operator Λ should be evaluated from the asymmetric prescription

$$\langle\tilde\Psi|\Lambda\,|\Psi\rangle = \langle\Phi|\tilde S\mathrm{e}^{-S}\Lambda\mathrm{e}^S|\Phi\rangle = \bar\Lambda(\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath)\,. \tag{14}$$

This recipe keeps trace of the artificial asymmetry as introduced in Eq. (13) which, in its turn, simplifies certain technical aspects of the global CCM approach. In particular, in the bi-variational spirit the energy expectation formula

$$\langle\tilde{\Psi}|H|\Psi\rangle = \langle\tilde{\Phi}|\hat{h}|\Phi\rangle \tag{15}$$

may now be minimized with respect to the full set of parameters $\{\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath\}$. Two equations follow, viz.,

$$\langle\Phi|C_\jmath^-\hat{h}|\Phi\rangle = 0\,; \quad \forall\jmath \neq 0 \tag{16}$$

and

$$\langle\Phi|\tilde{S}(\hat{h}-E)C_\jmath^+|\Phi\rangle = 0\,; \quad \forall\jmath \neq 0. \tag{17}$$

In their turn, these relations may be interpreted as a coupled algebraic set of equations that determine the parameters $\{\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath\}$. The consistency of the recipe may be reconfirmed by the derivation of the former relation (16) from the assumption of completeness of the set of states $\{\langle\Phi|C_\jmath^-\}$. Similarly, Eq. (17) may be perceived as a consequence of the completeness of the conjugate set $\{C_\jmath^+|\Phi\rangle\}$.

The coupled equations (16) and (17) are of the Goldstone linked-cluster type. For this reason, all extensive variables, such as the energy, scale linearly with the number of particles at every level of approximation. This is another merit of the CCM construction. Among the disadvantages we mention that the ground-state energy formula does not necessarily provide an upper bound, due to the intentional violation of manifest Hermiticity for the problem. Still, the recipe enables us to determine both the quickly convergent energies as well as the Hamiltonian-dependent values of parameters $\{\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath\}$ or, in various approximate schemes, of the respective truncated subsets of these values.

Within the general framework of the CCM treatment of many-body quantum systems some of the above-mentioned assumptions and restrictions may be removed. The method may certainly be extended, say, to cover also excited states and/or certain time-dependent versions of dynamics. In both of these directions, an implementation of ideas from THS context might prove particularly helpful.

3.2. CCM–THS correspondence

The close mathematical relationship between the various variational CCM recipes and the universal three-Hilbert-space (THS) representation of a generic quantum system has been largely overlooked till now. Apart from a few rather inessential differences, one of the key obstacles may be seen in the differences in their notations, a first sample of which is displayed in Table 1, where we see that for Hamiltonians, the CCM and THS notation conventions are strictly opposite (so we have to re-emphasize that in our present paper we are using the first-column notation conventions).

With due care paid to the Hermiticity or non-Hermiticity of the Hamiltonian, it seems equally important to spot the CCM - THS coincidences and/or differences in the definitions and meanings of the other concepts. For the ground-state wave functions, in particular, the parallels in the denotation of the same feature or quantity are displayed in Table 2.

An inspection of Table 2 reveals that in their respective current versions, the two formalisms are far from equivalent, indeed. At the same time, they may be both found to suffer of certain specific weak points. In fact, our present considerations were originally motivated precisely by a *parallel* analysis of these respective weaknesses. After their deeper study we came to the conclusion (documented and emphasized also by the above two respective compact reviews) that a perceivable profit might be gained by modifying and getting those two formalisms and/or methods of calculation closer to each other.

On the side of the CCM formalism, for example, one may immediately notice an obvious contrast between the exponential CCM form of the mapping $\Omega^{(CCM)} = \exp S^{(CCM)}$ and the manifestly *non-exponential*, polynomial form of the tilded operator $\tilde{S}$ entering the second CCM ansatz (9). Naturally, such a striking difference did not stay unnoticed in the related literature, and the idea has been implemented into the so called extended version of the CCM (ECCM) formalism [1, 2].

On the side of the general THS formalism, in parallel, we may now recollect one of the very popular formalism-simplifying tricks by which one works just with the special Hermitian mappings $\Omega_s = \Omega_s^\dagger = \exp S_s$ [11, 12]. Under this additional assumption one arrives at a fairly natural exponential form of the equally special but still sufficiently general subset of the positive-definite metrics, $\Theta_s = \exp 2S_s$. In this manner, after the respective replacements $\tilde{S} \to \tilde{S}^{(ECCM)}$ and $\Theta \to \Theta_s = \exp 2S_s$, the initially very different forms of the operators get closer.

Once one stops feeling discouraged by the similar, more or less purely formal differences, one has to reopen also the question of the respective roles of the operators $\tilde{S}$ and Θ in the purely numerical context. This is another type of difference which is, naturally, strongly dependent on the purpose of the calculation. Traditionally, the CCM and THS calculation purposes are truly rather different. Nevertheless, on the CCM side one immediately notices that the predominance of calculations of the ground-state characterstics does not exclude extensions, say, to the excited-state problem [18] or even to the description of systems which are allowed to exhibit a manifest time-dependence of their dynamics [19]. In this sense we are getting still closer to the respective time-independent and time-dependent non-Hermitian versions of the general and universal THS formulation of abstract quantum mechanics as summarized, say, in Refs. [4] and [5].

Ground state	**CCM [3]**	**THS [5]**
Purpose	bi-variationality	re-Hermitization of H in $\mathcal{H}^{(S)}$
Assumptions	$\tilde{S}$ = annihilation	$\Theta = \Omega^\dagger\Omega$, Ω = invertible
eigen-ket (simplified)	$\|\Phi\rangle$	$\|0\rangle \in \mathcal{H}^{(F,S)}$
eigen-bra (conjugate)	$\langle\Phi\|$	$\langle 0\| \in \mathcal{H}^{(F)\prime}$
eigen-bra (amended)	$\langle\tilde{\Phi}\| := \langle\Phi\|\tilde{S}$	$\langle\!\langle 0\| := \langle 0\|\Theta \ \in \mathcal{H}^{(S)\prime}$
microscopic ground state	$\|\Psi\rangle$	$\|0\succ \ = \Omega\|0\rangle \in \mathcal{H}^{(P)}$
first variational ansatz	$= e^S\|\Phi\rangle$	
left ground state	$\langle\tilde{\Psi}\|$	$\prec 0\| \ = \langle 0\|\Omega^\dagger = \langle\!\langle 0\|\Omega^{-1} \in \mathcal{H}^{(P)\prime}$
second variational ansatz	$= \langle\tilde{\Phi}\|e^{-S}$	

TABLE 2. Parallel notation conventions.

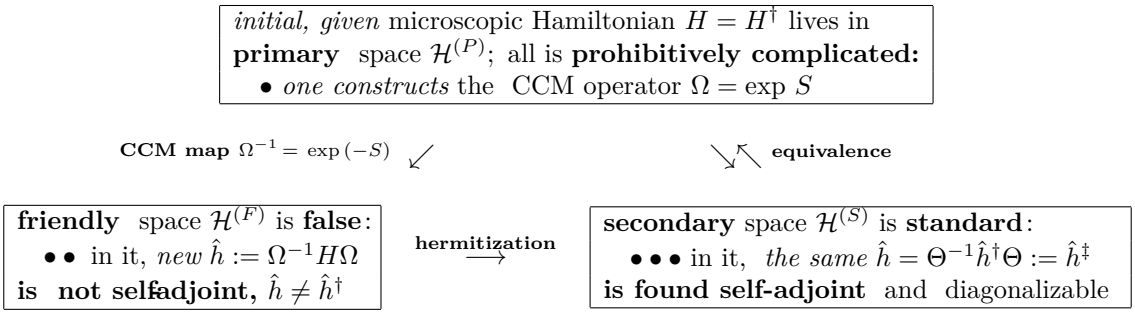

FIGURE 1. The three-Hilbert-space diagram.

4. Discussion

4.1. A CCM–THS fusion?

In the language of mathematics the core of our present message may be summarized as follows: in fact, it need not be particularly difficult to search for a further enhancement of parallels between the manifestly non-Hermitian, annihilation-operator-type CCM choice of the tilded operator $\tilde{S}$ and the strictly Hermitian and, in addition, also strictly positive definite Hilbert-space-metric operator $\Theta = \Omega^\dagger\Omega$. In the terminology of physics this persuasion is supported by the observation that what is *shared* by both the *abstract* CCM and THS formalisms is a truly exciting idea of using *nontrivial* "redundant" operators $\tilde{S}$ or Θ in place of the common identity operator.

In both formalisms, the rationale behind the use of the respective nontrivial operators $\tilde{S}$ and Θ is rather subtle though fairly persuasive and not too dissimilar. Indeed, one starts from a well known while, unfortunately, prohibitively complicated initial self-adjoint Hamiltonian in both cases (recall, once more, Table 1). Secondly, the choice and/or construction of the mapping $\Omega = \exp S$ is motivated, in both of the approaches, by a more or less comparably successful *simplification* of the Schrödinger eigenvalue problem. Thirdly, both the CCM and THS re-arrangements of the quantum bound-state problem lead to the necessity of the introduction of the respective nontrivial operators $\tilde{S}$ and Θ using *comparably strong* but, at the same time, *different* supportive arguments.

What now remains open is a truly challenging question as to whether, and in which sense, one could really achieve a *complete* coincidence of the respective (and, apparently, ideologically distant) CCM and THS recipes. Firstly, an affirmative answer may be given (and the idea may be made working) whenever the Hilbert spaces of the system remain, for whatever reason (e.g., for approximation purposes) finite-dimensional.

In such a very specific case the space for a compromise immediately opens after we move from the abstract formalism to any kind of a practical variational calculation and/or numerical approximation. Schematically speaking, any $2M$-parametric array of the multi-indexed CCM variational coefficients $\mathcal{S}_{\jmath_k}$ and $\tilde{\mathcal{S}}_{\jmath_k}$ with $k = 1, 2, \ldots, M$ may be perceived equivalent to an introduction of a $2M$-parametric metric $\Theta = \Omega^\dagger\Omega$. It should be noted, as a supportive argument, that even in the thorough IBM review [4] a large amount of space has been devoted to the study of finite-dimensional models and to the questions of practical variational applicability of the THS scheme.

On this level of mathematics the overall nature and structure of the above-indicated possibility of a complete unification (or, at least, of a strengthening of

the CCM–THS parallelism) may be read out of the three-Hilbert-space diagram in Figure 1. By the blobs we mark here the three main constructive CCM–THS steps. In the first two steps (viz., • and ••) we may assume to stay inside the usual CCM framework in which the ground-state eigenvector $|\Psi\rangle$ of the quantum system in question is reparametrized in terms of operator S. Thus, the CCM–THS innovation only emerges, via operators $\tilde{S}$ *alias* Θ, in the third step (• • •, see Table 2).

In this setting let us remind the readers that the (certainly, in general, existing) creation-operator components of $\Theta^{(CCM)}$ may be expected to play just a marginal role in the convergence. The reason is that the CCM choice of $\Omega = \exp S$ is mainly aimed at the construction of the many-body ground states. Thus, a lot of freedom is left for the introduction of more variational parameters via $\tilde{S} \neq I$. In contrast, the balanced distribution of attention of the universal THS formulae between the ground and excited states lowers, certainly, the latter freedom because the THS recipe defines the metric in terms of Ω unambiguously.

4.2. Towards the infinite-dimensional Hilbert spaces

Once we decide to leave the language of computing and once we move to the exact description of realistic quantum systems and to the (say, separable) infinite-dimensional Hilbert spaces, the search for the CCM–THS unification becomes perceivably more difficult. From the THS perspective, in particular, the key subtlety lies in the fact that whenever one decides to treat the two topological vector spaces $\mathcal{H}^{(P)}$ and $\mathcal{H}^{(F)}$ (naturally, still without any account of the definition of the inner products and of the metrics) as distinct, the map $\Omega = \exp S$ will slightly change its meaning as well as its interpretation.

From the alternative (and also historically older) CCM point of view it is necessary to recall, first of all, the results of the important paper [20]. Its author accepted the usual, above-described CCM linked-cluster parametrization, in its most general time-dependent form, as deduced from an appropriate action principle. In turn, this enforces a symplectic structure on the ensuing CCM phase space of the real-valued "degrees of freedom" $\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath$ of Eq. (14).

At this point the author of [20] has been forced to discuss the emergence of the characteristic non-Hermiticity of the average-value functionals $\bar{\Lambda}(\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath)$ of physical observables as well as of the action $\bar{\mathcal{A}}(\mathcal{S}_\jmath, \tilde{\mathcal{S}}_\jmath)$ itself.

In fact, our present idea of possible CCM–THS correspondence also found another source of inspiration in his approach, so let us recall his key ideas in more detail. Firstly, he introduced the set of complex conjugate variables $\mathcal{S}^*_\jmath, \tilde{\mathcal{S}}_\jmath{}^*$ and showed how they could be used to enlarge the CCM phase space into a genuine complex manifold but of too large a dimensionality. He further showed how the extra degrees of freedom could then be eliminated via the Dirac bracket technique. A set of constraint functions was introduced which thereby select the physical submanifold (*alias* the reduced phase space, or constraint surface) corresponding to the original Hilbert space. Subsequently, the reduced phase space was shown to be a (Kähler) complex manifold with a symplectic structure, just as the original extended one.

Ultimately, the Kähler manifold may be perceived as defining a positive, invertible, Hermitian geometry in the reduced phase space. Arponen [20] further shows that for a compound operator product $Q = \Lambda_1\Lambda_2$, the CCM star product which generates the expectation-value functional $\overline{Q} = \overline{\Lambda_1\Lambda_2}$ in terms of the individual expectation values $\overline{\Lambda_1}$ and $\overline{\Lambda_2}$, as given by Eq. (14), can be well defined in the reduced (i.e., physical) phase space.

This result suggests that besides starting from the THS scheme, one could also try to develop certain innovative and consequently Hermiticity-preserving hierarchical approximation schemes strictly within the CCM framework. A judicious use of the on-shell star products seems capable of establishing another form of the CCM–THS parallels, and of doing so in an entirely general setting. In addition, some explicit and concrete *constructive* implementations of the concept of the metric Θ may be found *directly* in the generic CCM framework. Naturally, a deeper analysis would require a verification in terms of explicit constructions. Further development of such a project lies, naturally, beyond the scope of our present paper.

4.3. Outlook

Let us summarize that in the general THS framework one is expected to perform all of the practical computations of physical predictions inside the "friendliest" Hilbert space $\mathcal{H}^{(F)}$. What is a real mathematical promise of a search for the new mutual CCM–THS correspondences is that even the standard probabilistic interpretation of many-body wave functions need not require a return to the "unfriendly" space $\mathcal{H}^{(P)}$. In all respects it becomes easier to replace the latter space by its (unitarily) equivalent alternative $\mathcal{H}^{(S)}$. The reason is that the latter Hilbert space only differs from its more friendly predecessor $\mathcal{H}^{(F)}$ by an *ad hoc* amended inner product.

Our present brief outline of a few explicit CCM–THS correspondences centered around the fact that operator $\tilde{S}$ of the CCM formalism coincides with the Hilbert-space metric operator Θ after a "translation of notation" to the THS-representation language of [5]. On the background of this comparison the main potential innovation of the CCM was found in the THS-based possibility of distinguishing between the *three* separate Hilbert spaces $\mathcal{H}^{(P)}$, $\mathcal{H}^{(F)}$ and $\mathcal{H}^{(S)}$, which would represent *the same* quantum many-body system.

The change of perspective revealed several CCM–THS parallels as well as differences. Among the par-

allels, one of the most inspiring seems to lie in the emerging structural similarity between the CCM constructions and their IBM (= interacting boson model) counterparts. The project of our future development of such a CCM–IBM correspondence seems promising. In the language of physics it might enable us to keep the initial physical P-superscripted Hilbert space as fermionic while rendering the other two, F- and S-superscripted Hilbert spaces, strictly in the generalized IBM spirit, carriers of another, generalized (e.g., pseudo-bosonic) statistics.

In the opposite direction, also the traditional IBM constructions of effective Hamiltonians could find some new inspiration in their CCM analogues. In particular, the prospects of a simplification mediated by the non-unitary invertible mappings $\Omega = \exp S$ need not necessarily stay bound by their traditional bosonic-image IBM restrictions. A new wealth of correspondences may be expected to become implementable between the auxiliary Hilbert space $\mathcal{H}^{(F)}$ and the, by assumption, prohibitively complicated physical Hilbert space $\mathcal{H}^{(P)}$ (hence, the superscript $^{(P)}$ may also mean "prohibitive").

Ultimately, the technically most productive idea may be seen in the exceptional role of the F-superscripted Hilbert space, in which the absence of an immediate physical interpretation (say, of the measurable aspects of coupled clusters) appears more than compensated by the optimal suitability of this particular representation space for calculations of the, typically, variational CCM type.

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